

# Scaling of nascent nodes in extended s-wave superconductors

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(Dated: January 20, 2013)

We analyze the low-energy properties of superconductors near the onset of accidental nodes, i.e. zeroes of the gap function not enforced by symmetry. The existence of such nodes has been motivated by recent experiments suggesting a transition between nodeless and nodal superconductivity in iron-based compounds. We find that the low-temperature behavior of the penetration depth, the specific heat, and the NMR-NQR spin-lattice relaxation rate are determined by the scaling properties of a quantum critical point associated with the nascent nodes. Although the power-law exponents are insensitive to weak short-range electronic interactions, they can be significantly altered by the curvature of the Fermi surface or by the three-dimensional character of the gap. Consequently, the behavior of macroscopic quantities near the onset of nodes can be used as a criterion to determine the nodal structure of the gap function.

After three years of their discovery, the symmetry of the superconducting state of the iron-based compounds is still under intense debate [1]. Although many early probes suggested a fully gapped state, recent experiments have found strong evidence for the presence of gapless quasi-particle excitations, suggesting the presence of nodes in at least some regions of the phase diagram [2–10]. Interestingly, in overdoped  $\text{Ba}(\text{Fe}_{1-x}\text{TM}_x)_2\text{As}_2$  materials, with  $\text{TM} = \text{Co, Ni, Pd}$ , penetration depth [2, 3], specific heat [6], and thermal conductivity measurements [4, 5] indicate a transition from a nodeless to an anisotropic nodal state, that does not seem to be related to changes in the Fermi surface (FS) topology. In underdoped  $(\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2$  compounds, where superconductivity (SC) may coexist with the magnetically ordered phase, recent thermal conductivity and penetration depth measurements also show a doping-induced onset of nodal quasi-particles [10, 11].

One possible scenario to explain these nodeless-to-nodal transitions is a change in symmetry from a SC state with finite gap everywhere on the FS, e.g. an isotropic s-wave pairing state, to a state with symmetry-enforced nodes, such as a d-wave state. In this case, a line of finite temperature phase transitions would separate the nodal and nodeless SC states. Indeed, for a range of band structure parameters, some theoretical models find nearly degenerate s-wave and d-wave solutions of the gap equations associated with purely electronic pairing interactions [12, 13]. Another scenario, not associated with a finite-temperature phase transition, is the emergence of accidental nodes, i.e. zeroes of the gap function at positions of the FS unrelated to a particular representation of the tetragonal symmetry group. In the iron pnictides, one frequently discussed gap function  $\Delta(\mathbf{k})$  is the extended s-wave, with different signs along different FS sheets [14–16]. The location of its zeroes in momentum space is determined by energetic arguments rather than symmetry requirements. Therefore, changing the size of the FS sheets or modifying quantitative details of the pairing interaction can cause such a zero to touch

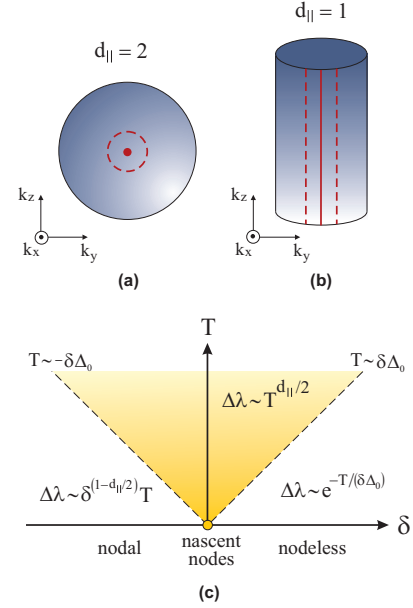


Figure 1: Accidental nodes in spherical (a) and cylindrical (b) Fermi surfaces. The point and the full line denote the  $\delta = 0$  nascent node in each case, whereas the dashed lines denote the line nodes that develop for  $\delta < 0$ .  $d_{||}$  is the number of directions on the FS with curvature. In (c) we present the  $T$ - $\delta$  phase diagram with the crossover regime (shaded yellow region between the dashed lines) and the scaling properties of the variation of the penetration depth  $\Delta\lambda$ .

and eventually cross one of the FS pockets, leading to a nodal state [18–28].

At finite temperatures, the onset of accidental nodes does not imply a phase transition. However, it is characterized by a quantum critical point (QCP) that separates a regime with finite-ranged quasi-particle excitations, in the fully gapped state, from a regime with algebraically decaying excitations, in the nodal state. Thus, general crossover arguments of QCP should be useful to characterize the behavior of macroscopic quantities near the onset of accidental nodes. Consider, for example, the varia-

tion of the penetration depth  $\Delta\lambda = \lambda(T) - \lambda(0)$  (we only consider the clean case here): in the gapped state one expects activated behavior,  $\Delta\lambda \propto \exp(-\Delta/T)$ , whereas in the case of line nodes holds  $\Delta\lambda = AT$ , with constant  $A$ . Naively, one expects that the transition between the two regimes is characterized by a power-law  $\Delta\lambda = A'T^n$  with exponent  $1 < n < \infty$  intermediate between the two regimes. For instance, if the accidental nodes first touch the FS at a single point, one would expect to observe  $n = 2$ , characteristic of systems with symmetry-enforced point nodes (see Ref.[29] for a review).

In this Brief Report we analyze the crossover behavior near the onset of accidental nodes and how it depends on the shape of the Fermi surface. Among others, our results demonstrate that even if nascent nodes originate around a single point, they behave qualitatively different from symmetry-enforced point nodes. Our main results are summarized in Fig.1: in the case of a spherical FS, at the onset of accidental nodes, we obtain a linear-in- $T$  penetration depth ( $n = 1$ ), but with a coefficient that is precisely half of the value that one finds for line nodes,  $A' = A/2$ . Consequently, after the onset of accidental nodes,  $\Delta\lambda$  displays a crossover between two linear-in- $T$  regimes with different slopes. Similar behaviors hold for other quantities, such as the specific heat  $C$  and the NMR-NQR spin-lattice relaxation rate  $T_1$ . In the case of a perfectly cylindrical Fermi surface we find, in agreement with earlier calculations [30], that  $n = 1/2$ , i.e. a behavior more singular even than for line nodes. Denoting by  $d_{\parallel}$  the number of directions on the FS with curvature ( $d_{\parallel} = 2$  for a spherical FS and  $d_{\parallel} = 1$  for a perfectly cylindrical FS), our results for the scaling behavior are expressed as  $\Delta\lambda \propto T^{d_{\parallel}/2}$ ,  $C \propto T^{1+d_{\parallel}/2}$ , and  $T_1^{-1} \propto T^{1+d_{\parallel}}$ . In order for the more exotic regime of cylindrical FS ( $d_{\parallel} = 1$ ) to be observed, the energy associated with the FS curvature must be negligible on the scale of the SC gap  $\Delta_0 \simeq 10$  meV, which is a very restrictive condition. Yet, this sensitivity with respect to the shape of the FS might enable one to distinguish between distinct nodal structures of the SC gap. In what follows, we will derive these results and show that they are robust against weak short range electron-electron interactions.

To describe the onset of accidental nodes we consider the angle-dependent gap function on the FS:

$$\frac{\Delta(\theta)}{\Delta_0} = \frac{1+\delta}{2} - \frac{1-\delta}{2} \cos(2\theta). \quad (1)$$

Here  $\Delta_0 > 0$  is the maximum amplitude of the gap,  $\theta$  is the angle measured relative to the center of the FS, and  $\delta$  is the tuning parameter. For  $\delta > 0$  the superconductor is fully gapped with minimum gap amplitude  $\Delta_0\delta$ . For  $\delta < 0$ , the gap function changes sign at nodes located at angles not fixed by symmetry,  $\theta_{0\pm} = \pm \frac{1}{2} \arccos\left(\frac{1+\delta}{1-\delta}\right)$ , and its most negative value is  $\Delta_0\delta < 0$ . The special case  $\delta = 0$  corresponds to the onset of nodes at  $\theta_0 = 0$

and  $\pi$ . Our results do not depend on the specific form of  $\Delta(\theta)$  given in Eq.1; rather, they apply generally to systems where, close to the nodes, the gap can be written as  $\Delta(\theta) \simeq \Delta_0(\theta + \theta_{0+})(\theta - \theta_{0-})$ . In this language, the QCP is characterized by the merging of the two nodes, giving rise to a quadratic dispersion  $\Delta(\theta) \simeq \Delta_0(\theta - \theta_0)^2$ . In the context of the iron pnictides,  $\theta$  in Eq.1 could be an angle relative to the center of the electron pocket. If one considers instead accidental nodes in the hole pocket, one simply replaces  $\cos(2\theta)$  by  $\cos(4\theta)$ , which does not change the results obtained here.

The low temperature behavior of numerous observables [29, 31] is determined by the density of states of Bogoliubov quasi-particles:

$$N(\omega) = N_0 \int d\varepsilon d\Omega \sum_{l=\pm 1} \delta\left(\omega - l\sqrt{\varepsilon^2 + \Delta(\theta)^2}\right), \quad (2)$$

where  $N_0$  is the normal-state density of states at the Fermi level and  $d\Omega$  refers to the angular integration. With  $N(\omega)$ , it is straightforward to obtain the temperature dependence of the penetration depth, the specific heat, and the NMR-NQR spin-lattice relaxation rate. Denoting the Fermi function by  $f(\omega) = (e^{\beta\omega} + 1)^{-1}$ , with  $\beta = (k_B T)^{-1}$ , one obtains:

$$\begin{aligned} \Delta\lambda &\propto \int_0^\infty d\omega N(\omega) \left(-\frac{\partial f(\omega)}{\partial \omega}\right), \\ C &\propto \int_0^\infty d\omega N(\omega) \beta \omega^2 \left(-\frac{\partial f(\omega)}{\partial \omega}\right), \\ \frac{1}{T_1 T} &\propto \int_0^\infty d\omega N(\omega)^2 \left(-\frac{\partial f(\omega)}{\partial \omega}\right). \end{aligned} \quad (3)$$

Band structure calculations as well as ARPES measurements reveal that the FS of the iron pnictides are anisotropic, similar in shape to warped cylinders [32]. Although small, this curvature of the FS becomes very relevant for the low energy properties of interest here. Thus, close to the accidental nodes, the FS is similar in shape to an ellipsoid which, upon rescaling, can be described by a sphere, yielding  $d\Omega = (4\pi)^{-1} \sin\theta d\theta d\varphi$  in Eq. 2. In this case the accidental line node becomes elliptical in shape, starting at an isolated point (see Fig.1a). The resulting density of states is given by:

$$N(\omega) = \frac{N_0}{\sqrt{1-\delta}} \int_{\max(\delta\Delta_0, -\omega)}^{\min(\Delta_0, \omega)} \frac{\omega}{\sqrt{\omega^2 - \Delta^2}} \frac{d\Delta}{\sqrt{\Delta_0 - \Delta}} \quad (4)$$

In Fig. 2, we show  $N(\omega)$  for  $\delta$  larger, smaller and equal to zero. At low energies  $|\omega| \ll \Delta_0$  and near the onset of nodes (i.e. for  $|\delta| \ll 1$ ), we obtain:

$$\frac{N(\omega)}{N_0} = \begin{cases} \frac{|\omega| \arccos\left(\frac{|\omega|}{\delta\Delta_0}\right)}{\Delta_0 \sqrt{1-\delta}} \Theta(|\omega| - \delta\Delta_0) & \delta > 0 \\ \frac{\pi}{2} \frac{|\omega|}{\Delta_0} & \delta = 0 \\ \frac{\pi}{\sqrt{1-\delta}} \frac{|\omega|}{\Delta_0} g\left(\frac{\omega}{|\delta|\Delta_0}\right) & \delta < 0 \end{cases} \quad (5)$$

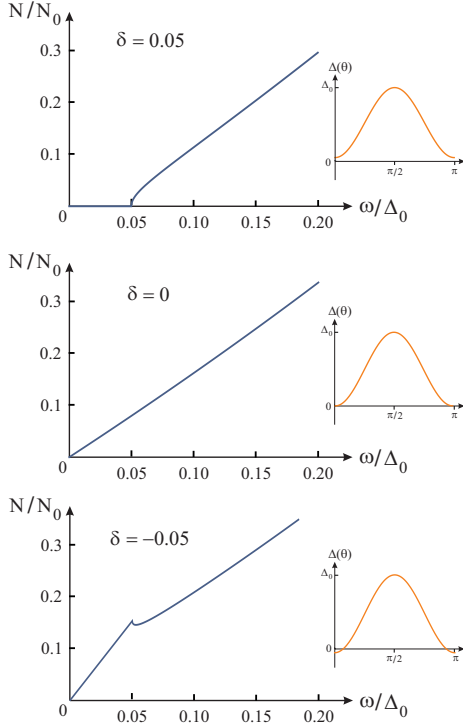


Figure 2: Density of states  $N$  as function of energy  $\omega$  in the case of a spherical Fermi surface for different values of  $\delta$ . The insets show the dependence of the gap  $\Delta$  on the polar angle  $\theta$ .

where  $g(x) = 1$  for  $|x| < 1$  and  $g(\omega) = \frac{1}{2} + \frac{1}{\pi} \arccot \sqrt{x^2 - 1}$  for  $|x| > 1$ . Notice that the nascent point nodes at  $\delta = 0$  behave differently than the symmetry enforced point nodes occurring in the polar state of triplet superconductors [29, 31]. In the latter, the gap magnitude near the node varies as  $|\theta - \theta_0|$ , as opposed to  $(\theta - \theta_0)^2$  discussed here, giving rise to  $N(\omega) \propto \omega^2$  instead of the  $N(\omega) \propto \omega$  found here. A similar result was discussed in Ref. [33], in the context of hybrid pairing states of uniaxial superconductors.

Because of the shallow rise of the gap near the nascent nodes, the slope of the density of states for  $\delta = 0$  is only half of the value for  $\delta < 0$ , where the gap actually changes sign. Consequently, for  $\delta < 0$  a crossover takes place between two regimes that are linear in  $\omega$ , with a low-energy slope twice as large as the higher-energy slope. In the fully gapped regime,  $\delta > 0$ , the density of states vanishes as  $N_0 \sqrt{\frac{2\delta}{1-\delta}} \sqrt{\frac{|\omega| - \delta\Delta_0}{\Delta_0}}$  near the threshold, but soon recovers the linear critical behavior at higher energies. This  $T = 0$  crossover regime is also manifested at finite temperatures, as we show in Fig. 3, where the  $T$ -dependence of the penetration depth is displayed for different values of the tuning parameter  $\delta$ . To probe the low-energy behavior of  $N(\omega)$ , low temperatures are required. Therefore, the observation of this crossover, or of a similar crossover in the slope of  $C/T$  or  $1/T^2 T_1$ ,

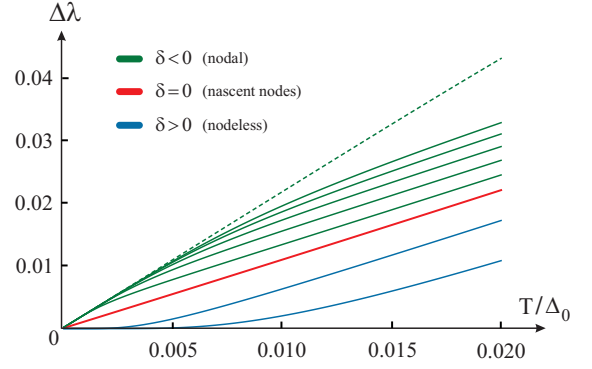


Figure 3: Variation of the penetration depth  $\Delta\lambda \equiv \lambda(T) - \lambda(0)$  as function of temperature  $T$  for several values of  $\delta$ . Notice in all curves the crossover at higher temperatures to the linear-in- $T$  dependence associated with the nascent nodes (solid red line). At low temperatures,  $\Delta\lambda$  decays exponentially for the fully gapped case (solid blue line) and linearly for the nodal case, but with a different slope (dashed green line). Here we used the values  $\delta = 0.025, 0.01, 0, -0.005, -0.01, -0.015, -0.02$ , and  $-0.025$ .

would be a strong evidence for accidental nodes and thus extended  $s$ -wave pairing.

For completeness, we also discuss the regime of perfectly cylindrical FS. In this case the angular integration becomes  $d\Omega = (2\pi)^{-1} d\theta$  and two nearly parallel line nodes emerge from a single line of nascent nodes with  $\Delta(\theta, k_z) \simeq \Delta_0 (\theta - \theta_0)^2$  independent of  $k_z$  (see Fig. 1b). The low-energy density of states is then given by

$$\frac{N(\omega)}{N_0} = \begin{cases} \left(\frac{2|\omega|}{\Delta_0}\right)^{1/2} \Theta(|\omega| - \delta\Delta_0) & \delta > 0 \\ 2(2\pi)^{-3/2} \Gamma\left(\frac{1}{4}\right)^2 \left(\frac{|\omega|}{\Delta_0}\right)^{1/2} & \delta = 0 \\ 2|\delta|^{-1/2} \frac{|\omega|}{\Delta_0} \tilde{g}\left(\frac{|\omega|}{\delta\Delta_0}\right) & \delta < 0 \end{cases} \quad (6)$$

with  $\tilde{g}(x) = 1$  for  $|x| \ll 1$ ,  $\tilde{g}(x) = (2\pi)^{-3/2} \Gamma\left(\frac{1}{4}\right)^2 |x|^{-1/2}$  for  $1 \ll |x| \ll |\delta|^{-1}$ , and a logarithmically diverging  $\tilde{g}(x) = \sqrt{2|\delta|/\pi^2} \log\left(\frac{1}{|x|-1}\right)$  close to  $x = 1$ . The surprising aspect of this result is that the power in  $N(\omega)$  at the QCP is lower even than the case of line nodes, a result that was obtained earlier in Ref. [30]. Thus, right at the transition to a fully gapped regime there are more low energy quasi-particle excitations compared to the nodal regime, again a consequence of the shallow rise of the gap for arbitrary  $k_z$ . Since the actual FS is not perfectly cylindrical, one expects a crossover to the linear in  $\omega$  behavior for a spherical FS, Eq. 5. This crossover will depend on details of the  $k_z$ -dispersions of the FS (as observed in [32]) and of the SC gap (as observed in [34, 35]) - in particular, on how the curvature of the FS changes as function of energy when compared to the changes in the SC gap. In Ref. [5], Reid *et al.* suggest the two nodal structures associated with Eqs. 5 and 6 as the

main candidates to explain their thermal conductivity measurements in overdoped  $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ . The different crossover behaviors of several macroscopic quantities that results from Eqs. 5 and 6 provide an important criterion to decide between the two scenarios.

The results above can also be obtained from scaling arguments of the low-energy action associated with the QCP. The free fermion action for  $\delta = 0$  is

$$S_0 = \int_k \psi_k^\dagger \begin{pmatrix} i\omega - vk_\perp & \alpha k_\parallel^2 \\ \alpha k_\parallel^2 & i\omega + vk_\perp \end{pmatrix} \psi_k \quad (7)$$

where we used the Nambu spinors  $\psi_k = (c_{k\uparrow}, c_{-k\downarrow}^\dagger)$  to denote the nodal quasi-particles. Here  $k = (k_\perp, \mathbf{k}_\parallel, i\omega)$  stands for momenta perpendicular and parallel to the FS measured from the location of the nascent node, with  $\int_k = T \sum_n \int dk_\perp d^d k_\parallel$ . Upon scaling  $k_\perp \rightarrow bk_\perp$ ,  $k_\parallel \rightarrow b^{1/2}k_\parallel$  and  $\omega \rightarrow b\omega$ , the action becomes scale invariant if one uses the rescaled field  $\psi_k = b^\kappa \psi'_k$  with  $\kappa = (6 + d_\parallel)/4$ . Thus, we find the scaling dimension of short range electron-electron interactions to be  $-d_\parallel/4$ . Since this scaling dimension is negative, weak short range electronic interactions are irrelevant in the sense of the renormalization group theory and should not lead to an instability. It remains to be analyzed the effects of long range interactions, such as quantum phase fluctuations.

Since the scaling dimension of the tuning parameter  $\delta$  is unity, we obtain the low-energy scaling form for the density of states:

$$N(\omega, \delta) = b^{-d_\parallel/2} N(b\omega, b\delta). \quad (8)$$

For  $\delta = 0$ , we can fix the arbitrary scaling parameter  $b = \omega^{-1}$  which yields  $N(\omega, 0) \propto \omega^{d_\parallel/2}$ . For finite  $\delta < 0$ , it holds that the slope  $A(\delta) = dN(\omega, \delta)/d\omega|_{\omega=0}$  behaves as  $A(\delta) \propto |\delta|^{1-d_\parallel/2}$ . These results are fully consistent with the explicit analysis presented above.

In summary, we analyzed the scaling behavior near the onset of accidental nodes in extended *s*-wave superconductors, and how it depends on the curvature of the FS. The low-*T* properties of the system can be analyzed in a simple scaling theory that is governed by a QCP separating a nodal and a nodeless region, without symmetry breaking. A somewhat similar behavior was proposed in extreme type-II superconductors, where the spectrum of Landau levels becomes gapless beyond a threshold magnetic field [36]. Our theory predicts that the low-temperature slope of the linear quasi-particle density of states at the onset of accidental nodes is reduced by a factor of 1/2 compared to the regime with well established nodes. This leads to an experimentally observable crossover in a number of physical observables, allowing one to distinguish whether nodes are accidental or symmetry enforced.

We thank A. V. Chubukov, R. T. Gordon, S. A. Kivelson, S. Maiti, R. Prozorov, J.-Ph. Reid, L. Taillefer, and M. Tanatar for useful discussions. Research at Ames Lab was supported by the U.S. DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

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